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UNCERTAINTY QUANTIFICATION OF COUPLED ODES WITH STOCHASTIC GALERKIN METHODS USING ADAPTIVE HIGHER ORDER RUNGE–KUTTA METHODS

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Abstract. Many real world problems are so complex that simplifications of these problems are needed. Otherwise the computing costs would be so high that specific problems, for example uncertainty quantification, could not be solved.

In this paper we consider a system of coupled ODEs and discretise the subsystems in time with adaptive high order Runge–Kutta methods. This approach is called "partitioned method", and we use a Block Gauss-Seidel method for solving the final linear or non-linear systems. The motivation for using high order methods is the computation of very accurate numerical results. Moreover, these time integration methods are more effective than lower order methods, and in the case of the partitioned approach they need less iterations than lower order methods.

For the stochastic discretisation we use a stochastic Galerkin method which only needs a few solutions of the deterministic ODE system. We show that using higher order methods in time leads to a better and more accurate quantification of uncertainties because we can expect a higher accuracy and a faster convergence for the deterministic problem. Numerical results show the advantages of the novel approach.

1 INTRODUCTION

Many physical or engineering problems can be described with differential equations, such as the simulation of time–dependent laminar or turbulent flows. As input quantities of such models we have, for example, boundary and initial conditions, geometries, and coefficients, which are in general not exactly known since they may be the result of measurements.

There are two kinds of uncertainties. First there are the so-called aleatoric uncertainties. Here the uncertainties are described as inherent randomness inside the phenomenon.

Then there are epistemic uncertainties which are related to our incomplete knowledge [17, 13, 29]. The uncertainties considered here are more or less epistemic uncertainties. Aleatoric uncertainties are nearly always described probabilistically [17, 13, 29, 9]. For epistemic uncertainties different ansatzes are used: Fuzzy systems, convex sets, intervals [22, 8, 29], as well as Bayesian probabilistic models [17, 13, 29, 6, 14].

The identified uncertainties should not only be indicated and verbally described by modelling and simulation, they should also be quantified (see for example [17]). The quantification of uncertainties plays an important role in the determination of optimal processes and to find feedback control which are robust with respect to perturbations and uncertainties. There are different possibilities to describe and quantify uncertainties. In this article uncertainties are described with probabilistic or stochastic models since this approach is based on a deep mathematical structure [17].

A good probabilistic description can be achieved, for example, with Gaussian random variables if the random variables are continuous. As Wiener suggests [32] every random variable $\mathsf{r}(\omega) \in L_2(\Omega)$ can be represented with polynomials, which depend on uncorrelated and independent Gauß variables [12, 16, 19, 20, 18]. This leads to functional approximations such as the polynomial chaos expansion (PCE), which delivers a suitable representation of the stochastic process and of the random variable in independent identically distributed (**iid**) standard-Gauß variables.

In this paper we consider linear coupled ODEs, where we assume that the initial conditions are uncertain. For the solution of this system of ODEs we need a temporal discretisation. Therefore we will concentrate on implicit schemes such as implicit Runge–Kutta methods, since a high order of convergence can be achieved (see [24]). Often an order reduction phenomenon can be observed if stiff problems or DAEs are solved (see [15] and [10]). Moreover, the costs for the linear algebra are very high. Therefore often diagonally implicit Runge-Kutta (DIRK) methods or Rosenbrock–Wanner (ROW) methods are used. But in this case the order reduction is much stronger. Many papers study the order reduction phenomena and derive further order conditions to reduce this effect. One possibility is the consideration of the Prothero–Robinson example [27]. In [23] and [26] better ROW methods are developed, and numerical studies show that full order can be achieved for the Prothero–Robinson example. Similar results for SDIRK and ESDIRK methods are presented in [23] and [25].

Here we want to use very accurate methods, i.e. methods which have a high order of convergence. Therefore fully implicit Runge–Kutta methods may be a good choice. But these methods need a high computational effort, since in every timestep a nonlinear system of dimension ns has to be solved, where n is the dimension of the problem and s is the number of internal stages of the Runge–Kutta method. In the last decades several papers have discussed the efficient solution of the nonlinear or linear equations. Here we use a transformation from Butcher [4] and Bickart [2] of the coefficient matrix of the Runge–Kutta method. If a simplified Newton method is applied this splitting leads to s complex valued systems of dimension n. An application of this technique for Radau

methods can be found in [11] and [28]. These nonlinear systems can be solved directly with the help of LU-decompositions and back- and forward substitutions.

For coupled ODEs such a discrete system can be very large, and a monolithic method may be not a good choice since the computations of the matrix-vector products need a lot of time and a lot of memory. A partitioned method may be a better choice. In this case we split the huge nonlinear system into smaller ones. This approach is known, for example, from the numerical solution of multi-field problems like fluid–structure interaction (see [21]).

This paper is structured as follows: First we discuss implicit Runge–Kutta methods and apply them on a coupled system of ODEs. Then stochastic Galerkin methods are presented, and finlly a numerical example shows the benefit of using higher order time integration methods.

2 TIME DISCRETISATION METHODS

We start our considerations with the initial value problem

$$\dot{\mathbf{u}} = \mathbf{f}(t, \mathbf{u}), \quad \mathbf{u}(t_0) = \mathbf{u}_0. \tag{1}$$

A Runge-Kutta (RK) method for the implicit ODE (1) is given by

$$\mathbf{k}_i = \mathbf{f}\left(t_m + c_i\tau, \mathbf{u}_m + \tau_m \sum_{j=1}^{s} a_{ij}\mathbf{k}_j\right), \quad i = 1, \dots, s, \tag{2}$$

$$\mathbf{u}_{m+1} = \mathbf{u}_m + \tau_m \sum_{i=1}^{s} b_i \mathbf{k}_i, \tag{3}$$

where τ is a given timestep size, s is the number of internal stages and a_{ij}, b_i, and c_i are the coefficients of the RK-method, which should be determined in such a way that the method has a sufficiently high order convergence [5, 10, 30]. The order of the RK-method can be determined with the so-called simplifying conditions from Butcher [3], which are defined as follows.

Definition 2.1 *(see [3]). An s-stage RK-method satisfies the simplifying conditions if the conditions*

$$\begin{aligned}
B(p): &\quad \sum_{i=1}^{s} b_i c_i^{k-1} &&= 1/k, && k = 1, \dots, p,\\
C(q): &\quad \sum_{j=1}^{s} a_{ij} c_j^{k-1} &&= c_i^k/k, && i = 1, \dots, s, k = 1, \dots, q,\\
D(r): &\quad \sum_{i=1}^{s} b_i c_i^{k-1} a_{ij} &&= b_j(1 - c_j^k)/k, && j = 1, \dots, s, k = 1, \dots, r
\end{aligned}$$

are fulfilled.

The condition $B(p)$ is equivalent to a quadrature rule with nodes c_i and weights b_i, which integrates polynomials of degree $p-1$ exactly. The conditions $C(q)$ have the following meaning: The intermediate values $\mathbf{k}_i$ are integrated exactly by a quadrature rule with weights a_{ij} and nodes c_i, which integrates polynomials of degree q exactly.

Theorem 2.2 *(see [5, 30]) An RK-method with s internal stages has the convergence order p if the simplifying conditions $B(p)$, $C(l)$, and $D(m)$ with*

$$p \leq \min\{l+m+1, 2l+2\}$$

are satisfied.

For the proof we refer to the book of Butcher [5]. Next we derive the coefficients of Radau-IIA methods, which need the roots of the shifted Legendre polynomial of degree s, i.e.

$$P_s(2t-1) = \frac{1}{s!}\frac{d^s}{dt^s}[t^s(t-1)^s].$$

With respect to the $L^2(0,1)$-scalar product the polynomial $P_s(2t-1)$ is orthogonal to all polynomials of degree $< s$. The roots of the Legrendre polynomials P_s can be found in the book of Abramowitz and Stegun [1] or can be computed with a computer algebra tool. It can be proven that the roots are pairwise distinct. From this fact it follows that the Vandermonde matrix

$$V_s = (V_{ij}) := (c_i^{j-1}) = \begin{pmatrix} 1 & c_1 & c_1^2 & \dots & c_1^{s-1} \\ \vdots & \vdots & \vdots & & \vdots \\ 1 & c_s & c_s^2 & \dots & c_s^{s-1} \end{pmatrix}, \qquad i,j = 1,\dots,s$$

is regular. In the case of the Radau methods we need the following theorem.

Theorem 2.3 *Let be given a Runge–Kutta method with $p = 2s-1$. Then the nodes c_i of the RK method are given by the roots of the polynomial*

$$P_{s,\xi}(2x-1) = P_s(2x-1) + \xi P_{s-1}(2x-1), \quad \xi \in \mathbb{R}.$$

For the proof we refer to the book of Strehmel and Weiner (see [31]). Here we are intested in the case $\xi = -1$, which leads to the Radau-IIA methods with $c_s = 1$ (see [7]). The condition $B(p)$ reads as $\mathbf{b}^\top \mathbf{c}^k = 1/k$, where the vector $\mathbf{c}^k$ is defined as $\mathbf{c}^k = (c_1^k, \dots, c_s^k)^\top$. The condition $C(q)$ can be written as $A\mathbf{c}^{k-1} = \mathbf{c}^k/k$, where $A = (a_{ij})_{i,j=1}^s$. The nodes b_i are then uniquely determined by the conditions $B(1)$, ..., $B(s)$, i. e. by

$$\mathbf{b}^\top \mathbf{e} = 1, \mathbf{b}^\top \mathbf{c} = 1/2, \dots, \mathbf{b}^\top \mathbf{c}^{s-1} = 1/s.$$

This system can be written in matrix-vector notation as

$$\mathbf{b}^\top V_s = \mathbf{e}_H^\top := \left(1, \frac{1}{2}, \dots, \frac{1}{s}\right).$$

Multiplying from the right with the inverse of V_s generates our nodes b_i, i.e. $\mathbf{b}^\top = \mathbf{e}_H^\top V_s^{-1}$. Next we determine the matrix A with the help of conditions $C(1), \ldots, C(s)$, which can be written as

$$A\mathbf{e} = \mathbf{c}, A\mathbf{c} = \mathbf{c^2}/2, \ldots, A\mathbf{c}^{s-1} = \mathbf{c^s}/s,$$

or in matrix notation by $AV_s = C$, where

$$C := (c_{ij}) = \frac{1}{j} c_i^j, \qquad i, j = 1, \ldots, s.$$

As it is shown in [24] the method can be equipped with an embedded method. Therefore we set

$$\tilde{\mathbf{e}}_H^\top := \left(1, \frac{1}{2}, \ldots, \frac{1}{s-1}, 0\right).$$

Then the nodes $\tilde{b}_i$ are given simply by

$$\tilde{\mathbf{b}}^\top = \tilde{\mathbf{e}}_H^\top V_s^{-1}$$

and the embedded method is of order $s-1$. Finally, the Butcher table is given by

$\mathbf{c}$	CV_s^{-1}
	$\mathbf{e}_H^\top V_s^{-1}$
	$\tilde{\mathbf{e}}_H^\top V_s^{-1}$

and the Radau-IIA methods with 2 and 3 internal stages are given by

$\frac{1}{3}$	$\frac{5}{12}$	$-\frac{1}{12}$
1	$\frac{3}{4}$	$\frac{1}{4}$
	$\frac{3}{4}$	$\frac{1}{4}$
	1	0

$\frac{4-\sqrt{6}}{10}$	$\frac{88-7\sqrt{6}}{360}$	$\frac{296-169\sqrt{6}}{1800}$	$\frac{-2+3\sqrt{6}}{225}$
$\frac{4+\sqrt{6}}{10}$	$\frac{296+169\sqrt{6}}{1800}$	$\frac{88+7\sqrt{6}}{360}$	$\frac{-2+3\sqrt{6}}{225}$
1	$\frac{16-6\sqrt{6}}{36}$	$\frac{16+6\sqrt{6}}{36}$	$\frac{1}{9}$
	$\frac{16-6\sqrt{6}}{36}$	$\frac{16+6\sqrt{6}}{36}$	$\frac{1}{9}$
	-1	$1-\frac{7}{12}\sqrt{6}$	$1+\frac{7}{12}\sqrt{6}$

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3 APPLICATION TO COUPLED ODEs

Let us consider a simple coupled ODE given by

$$\dot{\mathbf{u}} = \begin{pmatrix} a & b \\ -b & a \end{pmatrix} \mathbf{u}, \qquad \mathbf{u}(0) = \mathbf{u}_0. \tag{4}$$

In the following we solve the ODE (4) with a partitioned approach, where we use a Block Jacobi and a Block Gauss–Seidel method. The convergence of these partitioned methods

depends strongly on the spectral radius of the iteration matrix which depends on the Runge–Kutta method and on the chosen stepsize. The variables a and b in ODE (4) are set as follows: $a = -1/10$ and $b = 24$. As stepsizes we use $\tau = 1/10$ and $\tau = 1/100$. Note, that for $\tau = 1/10$ the implicit Euler and the trapezoidual rule do not converge if they are applied with a Block Jaboci or Block Gauss–Seidel method. In Figure 1 we show the results for Radau-IIA methods with $2, \ldots, 30$ internal stages. It can observed that

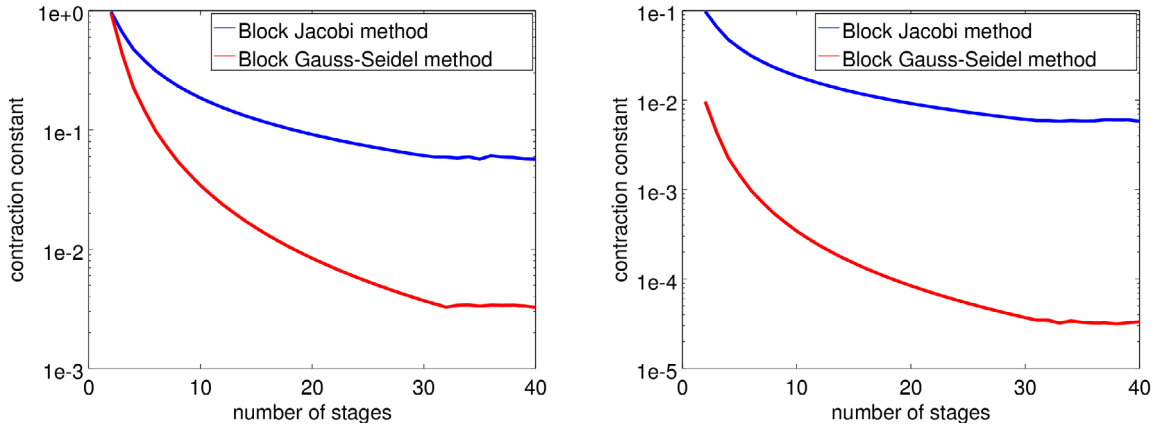

Figure 1: spectral radii in dependency of the internal stages with $\tau = 1/10$ (left) and $\tau = 1/100$ (right)

increasing the number of stages decreases the spectral radius, i.e. the numerical results are getting better and we need less iterations of our partitioned methods. Moreover, the spectral radius for the Block Gauss-Seidel method is lower than for the Block Jacobi method. The spectral radius can be reduced if the stepsize τ is reduced, because τ acts as a damping parameter.

In our next experiment we want to show that higher order methods need less iterations for the partitioned methods and that the numerical error decreases if the number of stages increases. Again we chose $a = -1/10$ and $b = 24$. For the stepsize we take $\tau = 1/10$. The numerical results are shown in Figure 2. In the left we plot the number of iterations for the partitioned methods in dependency of the number of internal stages. It can be observed that the lower order methods need much more iterations than the methods with 10 or more internal stages. A similar observation can be made if the numerical error is considered (left part of Figure 2). Again, methods with 10 or more stages have a smaller numerical error than lower order methods.

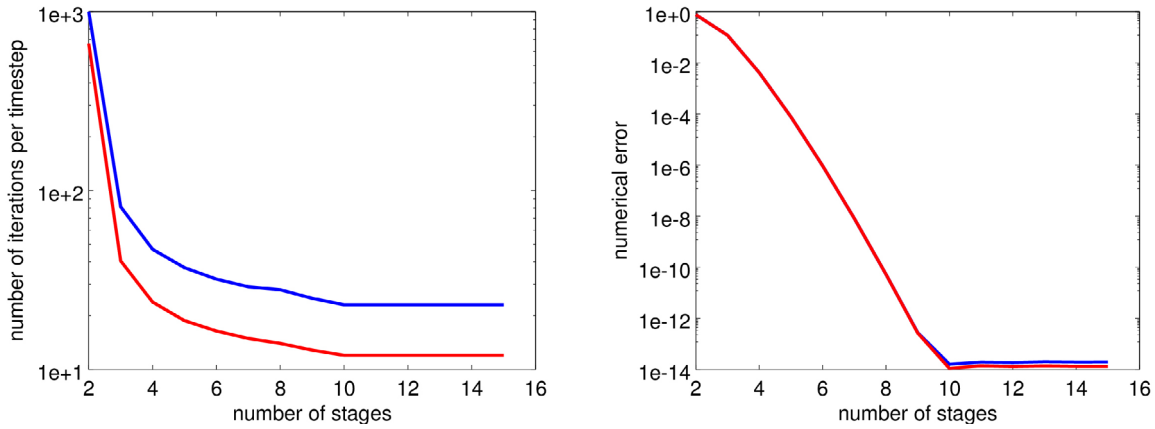

Figure 2: Iterations per timestep (left) and numerical error (right)

4 STOCHASTIC GALERKIN METHOD

In the next step we assume that the initial conditions of the ODE (4) are uncertain, i.e. we have a stochastic ODE given by

$$\dot{\mathbf{u}}(t,\omega) = \begin{pmatrix} a & b \\ -b & a \end{pmatrix} \mathbf{u}(t,\omega), \qquad \mathbf{u}(0,\omega) = \mathbf{u}_0(\omega), \tag{5}$$

where ω is an elementary event (of a realisation) in a probability space $(\Omega, \mathcal{A}, \mathbb{P})$ of random events. For the stochastic discretisation we use a Galerkin approach, i.e. we look for a variational formulation. Therefore we multiply equation (5) with a testfunction H_γ and integrate over the stochastic domain Ω. We receive

$$\int_\Omega \dot{u}(t,\omega) H_\gamma(\omega) \mathbb{P}(d\omega) = \int_\Omega \left[a u(t,\omega) + b v(t,\omega) \right] H_\gamma(\omega) \mathbb{P}(d\omega), \tag{6}$$

$$\int_\Omega \dot{v}(t,\omega) H_\gamma(\omega) \mathbb{P}(d\omega) = \int_\Omega \left[a v(t,\omega) - b u(t,\omega) \right] H_\gamma(\omega) \mathbb{P}(d\omega) \tag{7}$$

Any random variable $r(\omega) \in L_2(\Omega)$ can be represented as a series of polynomials in uncorrelated and independent Gaussian variables $\theta = (\theta_1, \dots)$ (see [32]). This idea is called *polynomial chaos expansion* (PCE). We set

$$u(t,\omega) = \sum_\alpha u_\alpha(t) H_\alpha(\theta(\omega)),$$

$$v(t,\omega) = \sum_\alpha v_\alpha(t) H_\alpha(\theta(\omega)).$$

For more details about we PCE we refer to [17]. Inserting these formulas into our variational formulation leads to the following system

$$\sum_\alpha \dot{u}_\alpha(t) \int_\Omega H_\alpha((\theta(\omega))H_\gamma(\omega)\mathbb{P}(d\omega) = \sum_\alpha u_\alpha(t)a \int_\Omega H_\alpha((\theta(\omega))H_\gamma(\omega)\mathbb{P}(d\omega) + \sum_\alpha v_\alpha(t)b \int_\Omega H_\alpha((\theta(\omega))H_\gamma(\omega)\mathbb{P}(d\omega), \tag{8}$$

$$\sum_\alpha \dot{v}_\alpha(t) \int_\Omega H_\alpha((\theta(\omega))H_\gamma(\omega)\mathbb{P}(d\omega) = \sum_\alpha v_\alpha(t)a \int_\Omega H_\alpha((\theta(\omega))H_\gamma(\omega)\mathbb{P}(d\omega) - \sum_\alpha u_\alpha(t)b \int_\Omega H_\alpha((\theta(\omega))H_\gamma(\omega)\mathbb{P}(d\omega). \tag{9}$$

The polynomials H_α are chosen in such a way that the integrals can be solved analytically. One choice are multivariate Hermite polynomials which can be defined with a recursion formula given by $h_{k+1}(t) = th_k(t) - kh_{k-1}$, $k \in \mathbb{N}$. The Hermite polynomials are orthogonal polynomials w.r.t. the standard Gaussian probability measure Γ, where $\Gamma(dt) = (2\pi)^{-1/2}e^{-t^2/2}$. The set $\{h_k(t)/\sqrt{k!} \mid k \in \mathbb{N}_0\}$ forms a complete orthonormal system in $L_2(\mathbb{R}, \Gamma)$, since the Hermite polynomials satisfy

$$\int_{-\infty}^{\infty} h_m(t)h_n(t)\Gamma(dt) = n!\delta_{nm}.$$

A multivariate Hermite polynomial is defined by

$$H_\alpha(\mathbf{t}) := \prod_{j=1}^{d} h_{\alpha_j}(t_j), \qquad \forall \mathbf{t} \in \mathbb{R}^d,$$

where α is a multi-index. In Figures 3 and 4 we have visualised the Hermite polynomials H_{23}, H_{33}, H_{35}, and H_{55}.

We can write each polynomial as a linear combination of Hermite polynomials. A product of two Hermite polynomials is again a polynomial which can be represented by Hermite polynomials, i. e.

$$h_k(t)h_l(t) = \sum_{n=|k-l|}^{k+l} c_{kl}^{(n)} h_n(t).$$

The coefficients $c_{kl}^{(n)}$ are only non-zero if $g := (k + l + n)/2 \in \mathbb{N}$ and if $g \geq k$, $g \geq l$ and $g \geq n$ (see [16]).

These properties of the Hermite algebra can be used to simplify equations (8)–(9). First of all we note that

$$\int_\Omega H_\alpha H_\gamma \mathbb{P}(d\omega) = \alpha!\delta_{\alpha\gamma}, \qquad \forall \alpha, \gamma$$

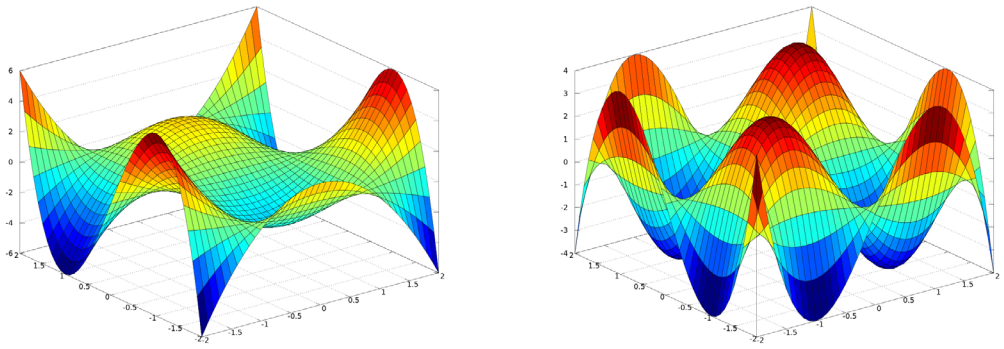

Figure 3: Hermite polynomials H_{23} and H_{33}

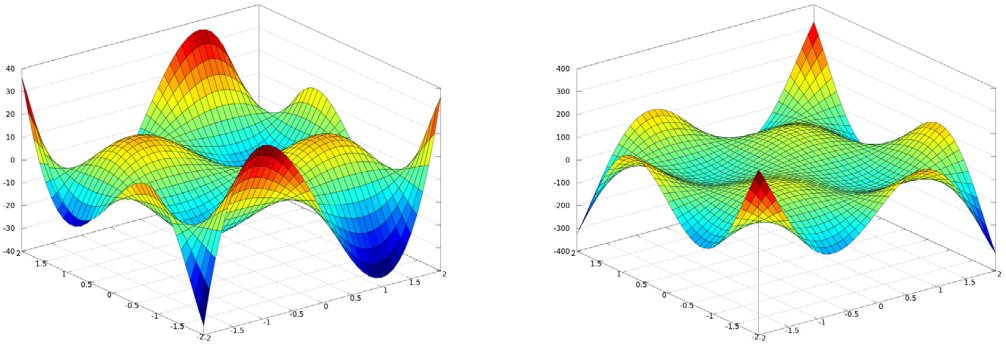

Figure 4: Hermite polynomials H_{35} and H_{55}

holds. If we use this result our stochastic ODE system simplifies to

$$\dot{u}_\alpha(t) = au_\alpha(t) + bv_\alpha(t), \tag{10}$$
$$\dot{v}_\alpha(t) = av_\alpha(t) - bu_\alpha(t). \tag{11}$$

This is a similar system as our deterministic system, i.e. we have to solve the original one with different initial values to compute the PCE.

5 NUMERICAL RESULTS

In our numerical example we consider the stochastic ODE (5). We solve this equation in the time interval $[0, 1]$ with Radau-IIA methods, where $s = 2, \ldots, 6$. From 1000 Monte Carlo runs the mean value and the variance is computed for the stochastic Galerkin method and the Monte Carlo method. The results are displayed in Figure 5. It can be observed that the results are more accurate if $s \geq 4$, i.e. if we use a Radau-IIA method of order 7. This observation holds for the stochastic Galerkin and the Monte Carlo method.

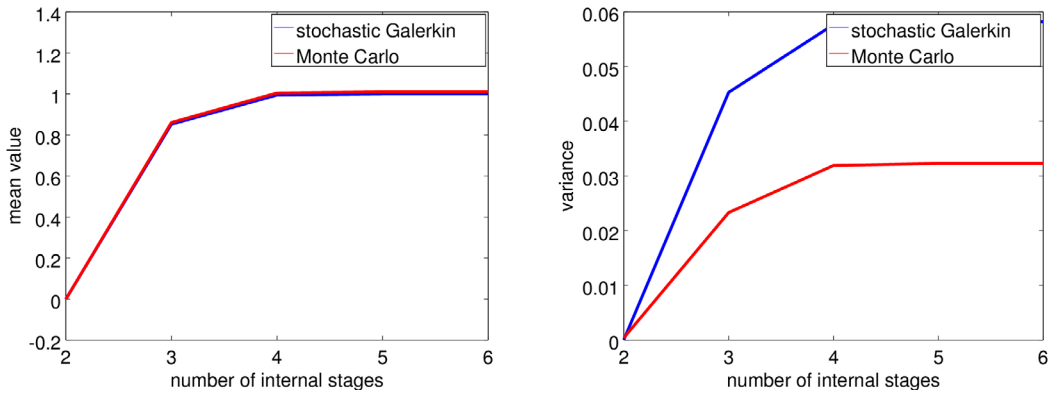

Figure 5: Results for the mean value (left) and the variance (right)

6 CONCLUSION

In this paper we have considered implicit Runge–Kutta methods of higher order and applied them on stochastic coupled ODEs. We have seen that in the case of deterministic problems a higher order leads to a smaller numerical error and higher order of convergence. Moreover a partitioned approach such as the Block Jacobi or the Block Gauss–Seidel method needs less iterations if the number of stages increases. This properties can be used for solving stochastic ODEs, too. We discretised our stochastic ODE with a stochastic Galerkin method, which in the case of stochastic initial conditions leads to a Block diagonal linear system, which can be easily solved.

In future work this approach should be applied on the model problem, where the matrix entries are uncertain, too. Moreover, a comparison with stochastic collocation methods should be carried out.

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